Spray Combustion Modeling Including Detailed Chemistry

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II. Structures of Spray Flames in the Counterflow Configuration

III. Turbulent Spray-Flame Modeling

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Modeling of Technical Spray Flames

Detailed Chemistry

Gas Phase

Droplet Vaporization

Drop Trajectories

Separated Flow
Why Detailed Chemistry?

Detailed Chemical Reaction Mechanisms are Available for a Considerate Number of Relevant Combustion Systems (Alcanes, Alcohols, Hydrogen/Air, Hydrogen/Oxygen, …)

• Combustion of liquid fuel sprays in air (e.g. internal engine combustion, industrial furnaces, gas turbine combustors)

• Liquid oxygen in (gaseous) hydrogen (liquid rocket propulsion)

• Liquid oxygen in gaseous hydrocarbons or alcohols (green propellants)
Advantages of Using Detailed Chemistry:

- Mechanism is independent of the experimental configuration, it depends only on pressure (not for hydrogen/air or hydrogen/oxygen)
- Mechanism is the base for development of reduced mechanisms (both manually or automatically developed systems)
- Prediction of pollutants and precursors of soot formation

Disadvantages of Using Detailed Chemistry:

- Stiffness of the conservation equations
- Consume a considerable amount of computer time

Applications:

Laminar Flames: Detailed mechanisms can be implemented directly for hydrogen and small hydrocarbons and alcohols
Turbulent Flames: Detailed chemistry may be implemented through use of the flamelet model
Modeling of Laminar Spray Flames in the Counterflow Configuration

**Motivation:**
Investigation of laminar spray flame structures using detailed models for instance for chemical reactions

Flamelet modeling of turbulent spray diffusion flames

**Properties:**
- Planar or axisymmetric
- Two-dimensional
- Strained
Detailed Versus One-Step Chemistry

n-Heptane/Air Spray Flame at Atmospheric Pressure

\( a = 500/s \)

**Detailed Chemistry:**

- Solid Lines, Square

**One-Step Chemistry:**

- Dashed Lines, Triangles

⇒ **One-Step Chemistry is not Suitable to Correctly Predict Even the Outer Flame Structure**

Mathematical Model

Gas-phase with dilute spray

- Boundary layer approximation, low Mach number
- Dimensionless, steady equations
- Similarity transformation $\Rightarrow$ 2D $\rightarrow$ 1D equations
- Ideal gas law
- Detailed chemical reaction mechanisms.
  - $\text{H}_2/\text{O}_2$ (8 species and 38 elementary reactions)
  - methanol/air (23 species and 170 elementary reactions)
- Detailed transport: molecular diffusion and thermo diffusion
- Gas-phase properties between 300 and 5000 K from NASA polynomials
- Physical properties of $\text{H}_2$ and $\text{O}_2$ in the range of 80 to 300 K and 1 to 200 bar from JSME tables
Mathematical Model

Liquid phase

- Mono-, bi- and polydisperse sprays, single-component sprays
- Discrete droplet model
- Spherically symmetric droplets
- Convective droplet model for heating and vaporization (Abramzon-Sirignano model)
- Pressure and temperature dependent heat of vaporization
- Assumption of thermodynamic equilibrium:
  - Ambrose’s equation for the evaluation of the vapor pressure for methanol/air
  - Calculation of binary H₂/O₂ mixtures to obtain the gas mixture composition at the interface (replacement of Raoult’s law)
- Droplet motion (drag)
Physical Properties of Oxygen (Cryogenic, High Pressure)

H₂/Air Spray Flame at Atmospheric Pressure

$p = 1$ bar, $T_\infty = T_\infty = 300$ K, $a = 100$/s


LOX/H\textsubscript{2} Spray Flame

\begin{itemize}
  \item **bidisperse**
  \item **monodisperse**
\end{itemize}

\begin{equation*}
  p = 30 \text{ bar}, \quad \Phi = 6, \quad a = 3,000/\text{s (spray side)}, \quad R_{A,0} = 10 \ \mu\text{m}, \quad R_{B,0} = 25 \ \mu\text{m}, \quad \text{SMR}_0 = 14.3 \ \mu\text{m}
\end{equation*}

LOX/H₂ Spray Flame

\[ p = 30 \text{ bar}, \ \Phi = 6, \ a = 3,000/\text{s (spray side)}, \ R_{A,0} = 10 \ \mu\text{m}, \ R_{B,0} = 25 \ \mu\text{m}, \ \text{SMR}_0 = 14.3 \ \mu\text{m} \]

LOX/H₂ Spray Flame

Chemical Reaction Rate and Vaporization Rate

\[ p = 30 \text{ bar}, \ \Phi = 6, \ a = 3,000/s \text{ (spray side)}, \ R_{A,0} = 10 \ \mu m, \ R_{B,0} = 25 \ \mu m, \ SMR_0 = 14.3 \ \mu m \]

Multiple Structures of Spray Flames

Methanol/Air Spray Flame at Atmospheric Pressure

\( a = 100/s \)

Multiple Structures of Spray Flames

Methanol/Air Spray Flame at Atmospheric Pressure

\[ a = 300/s \]

Methanol/Air Spray Flame at Atmospheric Pressure

\( a = 500/s \)

Multiple Structures of Spray Flames

Methanol/Air Spray Flame at Atmospheric Pressure

\[ a = 300/s \]

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Comparison: Gas-Sided Flame and Pure Gas Flames

Methanol/Air Spray Flame at Atmospheric Pressure

\[ a = 300/s \]

Methanol/Air Spray Flame at Atmospheric Pressure

Comparison of Spray and Gas Flame

Structures of Laminar Spray Flames in the Counterflow Configuration

• The LOX/H₂ Spray Flames are very stable and persist to strain rates of 25,000/s. The non-monotonicity of the gaseous oxygen profile on the spray side stems from the competition of vaporization and combustion.

• Multiple structures of methanol/air spray flames have been found for strain rates up to 400/s. The inner structure of the gas-sided flame is the same as a pure gas flamelet with appropriate initial conditions.

• At high strain, the gas-sided flame is extinguished and the spray-sided flame moves towards the gas-side of the counterflow configuration.

Question: How does the finding affect models such as the flamelet model for turbulent spray diffusion flames?
Flamelet-Model for Turbulent Diffusion Flames

Turbulent Flame

Library of laminar flame structures in the counterflow configuration

\[ \chi_1 \quad \chi_2 \quad \chi_3 \]

\[ \Phi_i = \Phi_i(\xi, \chi) \]

\[ \tilde{\Phi}_i = \int_0^\infty \int_0^1 \Phi_i(\xi; \chi) \tilde{P}(\xi) \tilde{P}(\chi) \, d\xi \, d\chi \]

- Gas flames
  - Strain rate
- Spray flames
  - Strain rate
  - Droplet size
  - Droplet velocity
  - Equivalence ratio
Laminar Spray Flame Structures for Use in Flamelet Models for Turbulent Spray Diffusion Flames (Methanol/Air)

Modeling of Turbulent Spray Flames

Replace by Pure Gas Flamelet

Turbulent Flow

All droplets vaporized $r_s < 1 \mu m$
Sauter Mean Radius $1 \mu m < r_s < 10 \mu m$
Sauter Mean Radius $10 \mu m < r_s < 25 \mu m$

Laminar Flow

Left Wing

Leads to Simplification of Implementing Laminar Spray Flamelets

$r_g = 10 \mu m$
$r_g = 25 \mu m$
Modeling of Turbulent LOX/H₂ Spray Flames

Micro Combustion Chamber M3 (DLR Lampoldshausen)

OH-Emission, $p = 5$ bar, $T_0 = 100$ K


Modeling of Turbulent Spray Flames

Mixing in Turbulent Sprays

- The $\beta$-function that is typically used to describe the mixing in turbulent diffusion flames does not perform well in regions where vaporization is present$^1$.

- **Here**: Modification of the description of the $\beta$-function through use of a transport equation for the probability density function of the mixture fraction, $\tilde{f}$, in turbulent sprays$^2$:

\[
\overline{\rho}_g \frac{\partial \tilde{f}}{\partial t} + \overline{\rho}_g U_j \frac{\partial \tilde{f}}{\partial x_j} + \frac{\partial (\overline{\rho}_g \overline{S}_s \tilde{f})}{\partial \zeta_c} = - \frac{\partial}{\partial \zeta_c} \left[ \overline{\rho}_g \left( \frac{\partial}{\partial x_j} \left( D_M \frac{\partial \zeta_c}{\partial x_j} \right) \right) \zeta_c \right] \tilde{f}.
\]


Mixing in Turbulent Methanol/Air Sprays

Methanol Vapor Fraction and PDF of the Mixture Fraction

Probability Density Functions at Various Positions

\[ P(\xi_c) = \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} \xi_c^{\alpha - 1} (1 - \xi_c)^{\beta - 1} \]

\[ P(\xi_c) = \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} (\xi_{c,\text{max}} - \xi_{c,\text{min}})^{1 - \alpha - \beta} (\xi_c - \xi_{c,\text{min}})^{\alpha - 1} (\xi_{c,\text{max}} - \xi_c)^{\beta - 1} \]

Comparison of Results with Presumed and Monte-Carlo PDF, and with Experiment

$x = 25 \text{ mm}$

$x = 50 \text{ mm}$


Summary and Conclusions

- LOX/H₂ spray flames in the counter-flow configuration have been studied, and the gaseous oxygen profile shows a non-monotonic behavior because of the high reactivity of the system. The flames persist to strain rates up to 25,000/s, and extinction has not yet been found.

- Multiple structures of laminar methanol/air counter-flowing spray flames have been identified at low strain rates up to 400/s on the spray side of the configuration for the present conditions. The gas-sided spray flame shows the same inner structure as a pure gas flamelet with appropriate boundary conditions, and this simplifies the implementation of the flamelet model for turbulent spray diffusion flames.

- The assumed $\beta$-function for the turbulent mixing in spray flames is poor in regions where vaporization exists, and it has been replaced by a PDF transport equation for the mixture fraction. A modified $\beta$-function is suitable to predict the shape of the PDF of the mixture fraction.
Future Research

- Extension of the model to unsteady flamelets
- Application of the PDF method to turbulent spray flame simulations
- Extension to other liquids